

LECTURE NOTES ON PHS 473: COMPUTATIONAL PHYSICS

BY

DR V.C. OZEBO

CONTENT

- Use of numerical methods in Physics
- Various methods of numerical differentiation and integration
- Numerical solution of some differential equations of interest in Physics
- Statistical analysis of data

CHAPTER ONE

ERRORS

An error may be defined as the difference between an exact and computed value,

Suppose the exact value of a solution of a computational problem is 1.023; now when a computer or calculator is used, the solution is obtained as 1.022823; hence the error in this calculation is $(1.023 - 1.022823) 0.000177$

Types of Error

Round-off error:- This error due to the rounding-off of a quantity due to limitations in the digits.

Truncation error:- Truncation means cutting off the other digits i.e. no rounding –off. For instance, 1.8123459 may be truncated to 1.812345 due to a preset allowable number of digits.

Absolute Error:- The absolute value of an error is called the absolute error; that is;

$$\text{Absolute error} = |error|$$

Relative error:- Relative error is the ratio of the absolute error to the absolute value of the exact value.; That is

$$\text{Relative error} = \frac{\text{Absolute error}}{|\text{exact value}|}$$

Percentage error:- This is equivalent to Relative error $\times 100$

Inherent error:- In a numerical method calculation, we may have some basic mathematical assumptions for simplifying a problem. Due to these assumptions, some errors are possible at the beginning of the process itself. This error is known as inherent error.

Accumulated error:- Consider the following procedure:

$$Y_{i+1} = 100Y_i \quad (i = 0, 1, 2, \dots)$$

Therefore,

$$Y_1 = 100Y_0$$

$$Y_2 = 100Y_1$$

$$Y_3 = 100Y_2 \text{ etc}$$

Let the exact value of $Y_0 = 9.98$

Suppose we start with $Y_0 = 10$

Here, there is an inherent error of 0.02

Therefore,

$$Y_1 = 100Y_0 = 100 \times 10 = 1000$$

$$Y_2 = 100Y_1 = 100 \times 1000 = 100,000$$

$$Y_3 = 100Y_2 = 100 \times 100,000 = 10,000,000$$

The table below shows the exact and computed values,

Variable	Exact Value	Computed value	Error
Y_0	9.98	10	0.02
Y_1	998	1000	2
Y_2	99800	100,000	200
Y_3	9980000	10,000,000	20,000

Notice above, how the error quantities accumulated. A small error of 0.02 at Y_0 leads to an error of 20,000 in Y_3 . So, in a sequence of computations, an error in one value may affect the computation of the next value and the error gets accumulated. This is called accumulated error.

Relative Accumulated Error

This is the ratio of the accumulated error to the exact value of that iteration. In the above example, the relative accumulated error is shown below.

Variable	Exact Value	Computed value	Accumulated Error	Relative Accumulated error
Y_0	9.98	10	0.02	$0.02/9.98 = 0.002004$
Y_1	998	1000	2	$2/998 = 0.002004$
Y_2	99800	100,000	200	$200/99800 = 0.002004$
Y_3	9980000	10,000,000	20,000	$20,000/9980000 = 0.002004$

Notice that the relative accumulated error is same for all the values.

CHAPTER TWO

ROOT FINDING IN ONE DIMENSION

This involves searching for solutions to equations of the form: $F(x) = 0$

The various methods include:

1. *Bisection Method*

This is the simplest method of finding a root to an equation. Here we need two initial guesses x_a and x_b which bracket the root.

Let $F_a = f(x_a)$ and $F_b = f(x_b)$ such that $F_a F_b \leq 0$ (see fig 1)

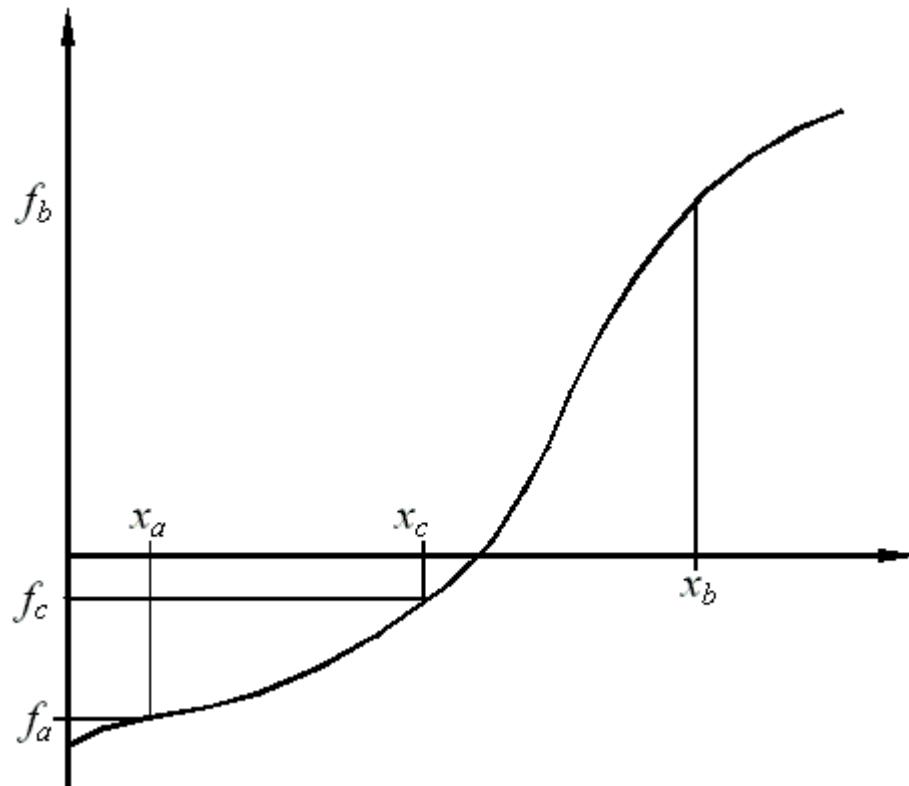


Figure1: Graphical representation of the bisection method showing two initial guesses (x_a and x_b bracketting the root).

Clearly, if $F_a F_b = 0$ then one or both of x_a and x_b must be a root of $F(x) = 0$

The basic algorithm for the bisection method relies on repeated applications of:

$$\text{Let } x_c = \frac{(x_a + x_b)}{2}$$

If $F_c = f(c) = 0$ then, $x = x_c$ is an exact solution,

Else if $F_a F_b < 0$ then the root lies in the interval (x_a, x_c)

Else the root lies in the interval (x_c, x_b)

By replacing the interval (x_a, x_b) with either (x_a, x_c) or (x_c, x_b) (whichever brackets the root), the error in our estimation of the solution to $F(x) = 0$ is on the average, halved.

We repeat this interval halving until either the exact root has been found or the interval is smaller than some specified tolerance.

Hence, the root bisection is a simple but slowly convergent method for finding a solution of $F(x) = 0$, assuming the function f is continuous. It is based on the intermediate value theorem, which states that if a continuous function f has opposite signs at some $x = a$ and $x = b (> a)$ that is, either $f(a) < 0, f(b) > 0$ or $f(a) > 0, f(b) < 0$, then f must be 0 somewhere on $[a, b]$.

We thus obtain a solution by repeated bisection of the interval and in each iteration, we pick that half which also satisfies that sign condition.

Example:

Given that $F(x) = x - 2.44$, solve using the method of root bisection, the form

$$F(x) = 0 .$$

Solution:

Given that $F(x) = x - 2.44 = 0$

Therefore,

$$x - 2.44 = 0$$

Direct method gives $x = 2.44$

But by root bisection;

Let the trial value of $x = -1$

X	F(x) = x-2.44
Trial value	
-1	-3.44
0	-2.44
1	-1.44
2	-0.44
3	+0.56

It is clear from the table that the solution lies between $x = 2$ and $x = 3$.

Now choosing $x = 2.5$, we obtain $F(x) = 0.06$, we thus discard $x = 3$ since $F(x)$ must lie between 2.5 and 2. Bisecting 2 and 2.5, we have $x = 2.25$ with $F(x) = -0.19$.

Obviously now, the answer must lie between 2.25 and 2.5.

The bisection thus continues until we obtain $F(x)$ very close to zero, with the two values of x having opposite signs.

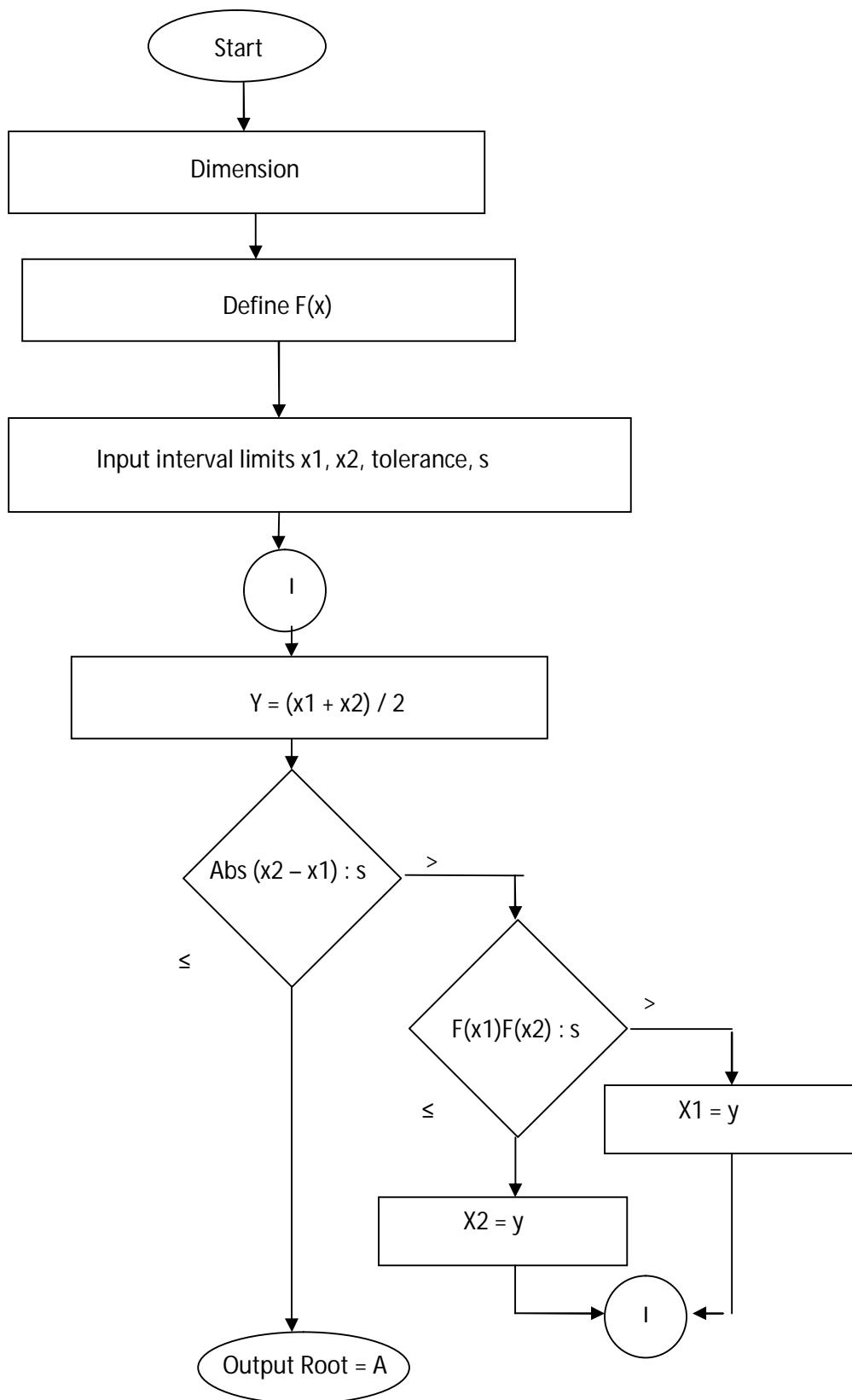
X	F(x) = x-2.44
2.25	-0.19
2.375	-0.065
2.4375	-0.0025
2.50	-0.06

When the above is implemented in a computer program, it may be instructed to stop at say, $|F(x)| \leq 10^{-4}$, since the computer may not get exactly to zero.

Full Algorithm

1. Define $F(x)$
2. Read x_1, x_2 , values of x such that $F(x_1)F(x_2) < 0$
3. Read convergence term, $s = 10^{-6}$, say.
4. Calculate $F(y)$, $y = (x_1+x_2) / 2$
5. If $\text{abs}(x_2-x_1) \leq s$, then y is a root. Go to 9
6. If $\text{abs}(x_2-x_1) > s$, Go to 7
7. If $F(x_1)F(x_2) \leq 0$, (x_1, y) contains a root, set $x_2 = y$ and return to step 4
8. If not, (y, x_2) contains a root, set $x_1 = y$ and return to step 4
9. Write the root A

Flowchart for the Root Bisection Method



2. The RegulaFalsi (False position) Method

This method is similar to the bisection method in the sense that it requires two initial guesses to bracket the root. However, instead of simply dividing the region in two, a linear interpolation is used to obtain a new point which is (hopefully, but not necessarily) closer to the root than the equivalent estimate for the bisection method. A graphical interpretation of this method is shown in figure 2.

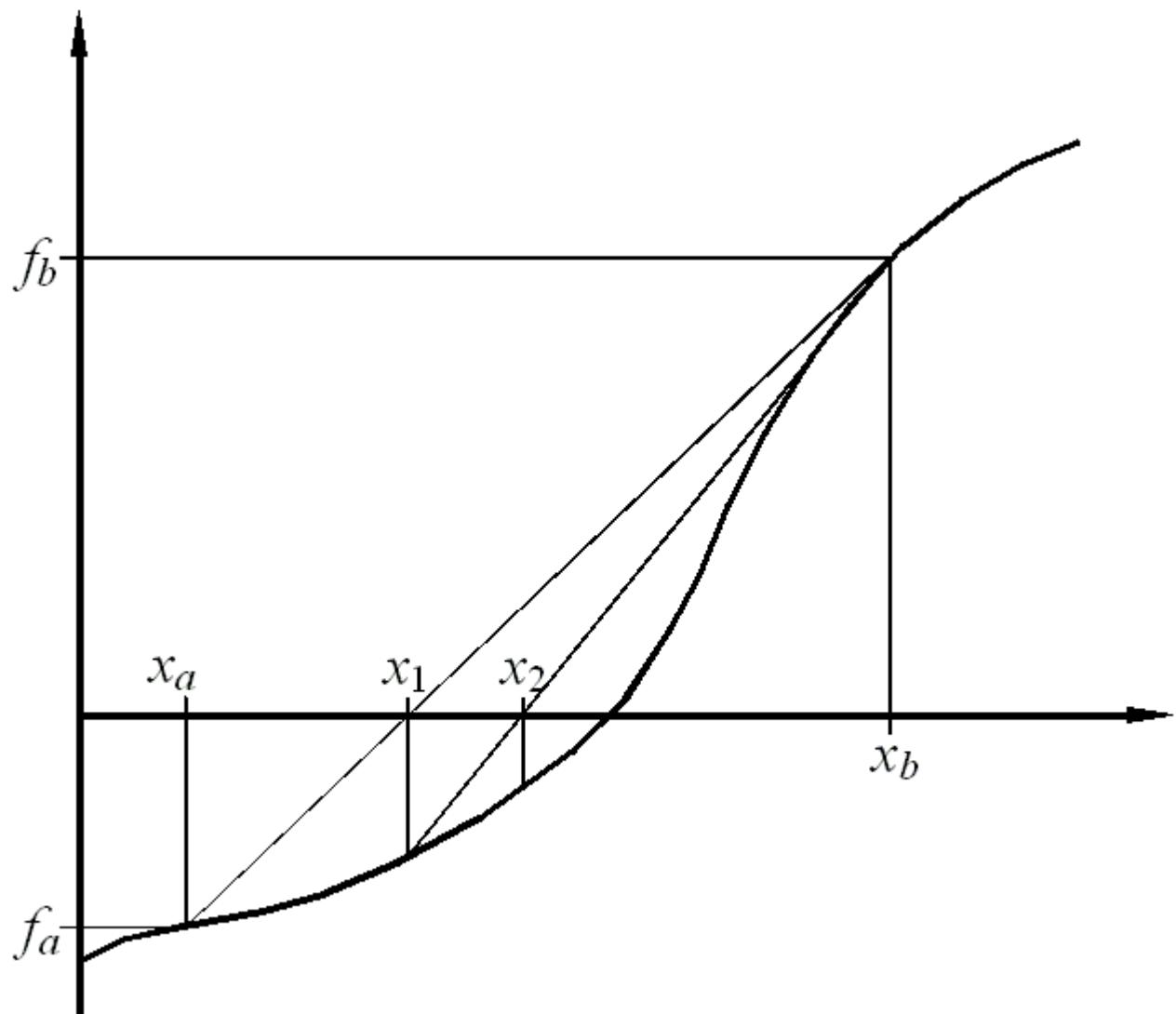


Figure 2: Root finding by the linear interpolation (regulafalsi) method. The two initial guesses x_a and x_b must bracket the root.

The basic algorithm for the method is:

$$\begin{aligned} \text{Let } x_c &= x_a - \frac{x_b - x_a}{f_b - f_a} f_a = x_b - \frac{x_b - x_a}{f_b - f_a} f_b \\ &= \frac{x_a f_b - x_b f_a}{f_b - f_a} \end{aligned}$$

If $f_c = f(x_c) = 0$ then $x = x_c$ is an exact solution..

Else if $f_a f_c < 0$ then the root lies in the interval (x_a, x_c)

Else the root lies in the interval (x_c, x_b)

Because the solution remains bracketed at each step convergence is guaranteed as was the case for bisection method, The method is first order and is exact for linear f

Note also that the method should not be used near a solution.

Example

Find all real solutions of the equation $x^4 = 2$ by the method of false position.

Solution

Let $x_a = 1$ and $x_b = 2$

Now rewriting the equation in the form: $x^4 - 2 = 0$

Then $f_a = 1^4 - 2 = -1$

$f_b = 2^4 - 2 = 14$

Therefore,

$$x_c = \frac{x_a f_b - x_b f_a}{f_b - f_a} = \frac{(1)(14) - (2)(-1)}{14 - (-1)} = \frac{16}{15} = 1.07$$

$$f_c = (1.07)^4 - 2 = -0.689$$

Now, from the algorithm, $f_c \neq 0$, hence $x_c \neq x$, the exact solution.

Again, $f_a f_b = (-1)(-0.689) = 0.689 > 0$

Therefore, the roots lie in the interval x_c, x_b

That is, $\pm(1.07, 2)$ (two roots)

3. The Newton-Raphson Method

This is another iteration method for solving equations of the form: $F(x) = 0$, where f is assumed to have a continuous derivative f' . The method is commonly used because of its simplicity and great speed. The idea is that we approximate the graph of f by suitable tangents. Using an approximate value x_0 obtained from the graph of f , we let x be the point of intersection of the x – axis and the tangent to the curve of f at x_0 .

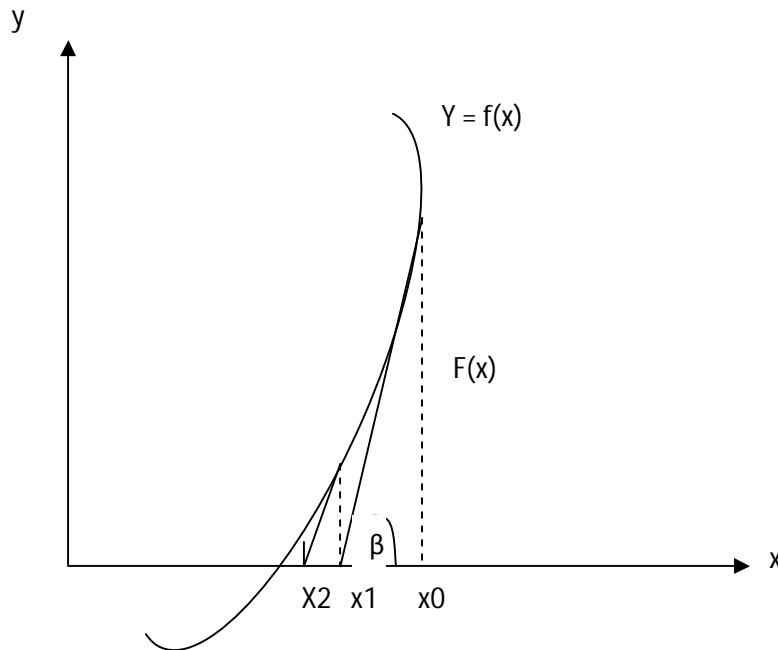


Figure 4: Illustration of the tangents to the curve in Newton-Raphson method

Then,

$$\tan \beta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1},$$

Hence,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)},$$

In the second step, we compute; $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$,

And generally,

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

Algorithm for the Newton-Raphson method

1. Define $f(x)$
2. Define $f'(x)$
3. Read x_0, s (tolerance0)
4. $K = 0$
5. $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)},$
6. Print $k+1, x_{k+1}, f(x_{k+1})$
7. If $|x_{k+1} - x_k| < s$ then go to 10
8. $K = k+1$
9. Go to step 5
10. Print ‘The root is ----‘, x_{k+1}
11. End

Consider the equation: $x^3 + 2x^2 + 2.2x + 0.4 = 0$

Here,

$$f(x) = x^3 + 2x^2 + 2.2x + 0.4$$

$$f'(x) = 3x^2 + 4x + 2.2$$

Let the initial guess, $x_0 = -0.5$

Let us now, write a FORTRAN program for solving the equation, using the Newton-Raphson’s method.

C NEWTON RAPHSON METHOD

DIMENSION X(100)

F(X) = X**3. + 2. *X*X + 2.2 *X + 0.4

F1(X) = 3. *X*X + 4. *X + 2.2

WRITE (*,*) 'TYPE THE INITIAL GUESS'

READ (*,5) X(0)

5 FORMAT (F10.4)

WRITE (*,*) 'TYPE THE TOLERANCE VALUE'

READ (*,6) S

6 FORMAT (F3.6)

WRITE (*,*) 'ITERATION X F(X)'

K = 0

50 X(K+1) = X(K) - F(X(K)) / F1(X(K))

 WRITE (*,10) K+1, X(K+1), F(X(K+1))

10 FORMAT (1X, I6, 5X, F10.4, 5X, F10.4)

 IF (ABS(X(K+1) - X(K)) .LE. S) GOTO 100

 K = K+1

 GOTO 50

100 WRITE (*,15) X(K+1)

15 FORMAT (1X, 'THE FINAL ROOT IS ', F10.4)

 STOP

 END

Assignment

If $S = 0.00005$, manually find the root of the above example after 5 iterations.

CHOOSING THE INITIAL GUESS, x_0

In the Newton-Raphson's method, we have to start with an initial guess, x_0 . How do we choose x_0 ?

If $f(a)$ and $f(b)$ are of opposite signs, then there is at least one value of x between a and b such that $f(x) = 0$. We can start with $f(0)$, find $f(0), f(1), f(2) \dots$. If there is a number k such that $f(k)$ and $f(k+1)$ are of opposite signs then there is one root between k and $k+1$, so we can choose the initial guess $x_0 = k$ or $x_0 = k+1$.

Example;

Consider the equation: $x^3 - 7x^2 + x + 1 = 0$

$$F(0) = 1 \text{ (= +ve)}$$

$$F(1) = -4 \text{ (= -ve)}$$

Therefore, there is a root between 0 and 1, hence our initial guess x_0 , may be taken as 0 or 1

Example:

Evaluate a real root of $x^3 + 2.1x^2 + 13.1x + 22.2 = 0$, using the Newton Raphson's method, correct to three decimal places.

Solution;

$$F(x) = x^3 + 2.1x^2 + 13.1x + 22.2$$

$$F(0) = 22.2 \text{ (positive)}$$

Now, since all the coefficients are positive, we note that $f(1), f(2), \dots$ are all positive. So the equation has no positive root.

We thus search in the negative side:

$$F(-1) = 20.2 \text{ (positive)}$$

$F(-2) = +ve = f(-3) ----- f(-11)$. But $f(-12)$ is negative, so we can choose $x_0 = -11$.

Iteration 1

$$F(x) = x^3 + 2.1x^2 + 13.1x + 22.2$$

$$F'(x) = 3x^2 + 24.2x + 13.1$$

Now, with $x_0 = -11$

$$F(x_0) = F(-11) = 11.2$$

$$F'(x_0) = F'(-11) = 3(-11)^2 + 24.2(-11) + 13.1 = 109.9$$

Therefore,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = -11 - \frac{11.2}{109.9} = -11.1019$$

Iteration 2

$$X_1 = -11.1019$$

$$F(x_1) = f(-11.1019) = -0.2169$$

$$F'(x_1) = F'(-11.1019) = 114.1906$$

Therefore,,

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -11.1019 - \frac{(-0.2169)}{114.1906} = -11.100001$$

Iteration 3

$$X_2 = -11.100001$$

$$F(x_2) = F(-11.100001) = -0.0001131$$

$$F'(x_2) = F'(-11.100001) = 114.1101$$

Therefore,

$$x_3 = x_2 - \frac{f(x_2)}{f'(x_2)} = -11.100001 - \frac{(-0.000113)}{114.1101} = -11.100000$$

Now, correct to three decimal places, $x_2 = x_3$, and so, the real root is $x = -11.100$.

Example 2

Set up a Newton-Raphson iteration for computing the square root x of a given positive number c and apply it to $c = 2$

Solution

We have $x = \sqrt{c}$, hence

$$F(x) = x^2 - c = 0$$

$$f'(x) = 2x$$

Newton-Raphson formula becomes:

$$\begin{aligned} x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{(x_k^2 - c)}{2x_k} \\ &= \frac{2x_k^2 - x_k^2 + c}{2x_k} = \frac{x_k^2 + c}{2x_k} \\ &= \frac{1}{2} \left(x_k + \frac{c}{x_k} \right) \end{aligned}$$

Therefore,

For $c = 2$, choosing $x_0 = 1$, we obtain:

$$X_1 = 1.500000, x_2 = 1.416667, x_3 = 1.414216, x_4 = 1.414214, \dots$$

Now, x_4 is exact to 6 decimal places.

Now, what happens iff $f'(x_k) = 0$?

Recall, if $f(x) = 0$, and $f'(x) = 0$, we have repeated roots or multiplicity (multiple roots). The sign in this case will not change; the method hence breaks down. The method also fails for a complex solution (i.e. $x^2 + 1 = 0$)

4. The Secant Method

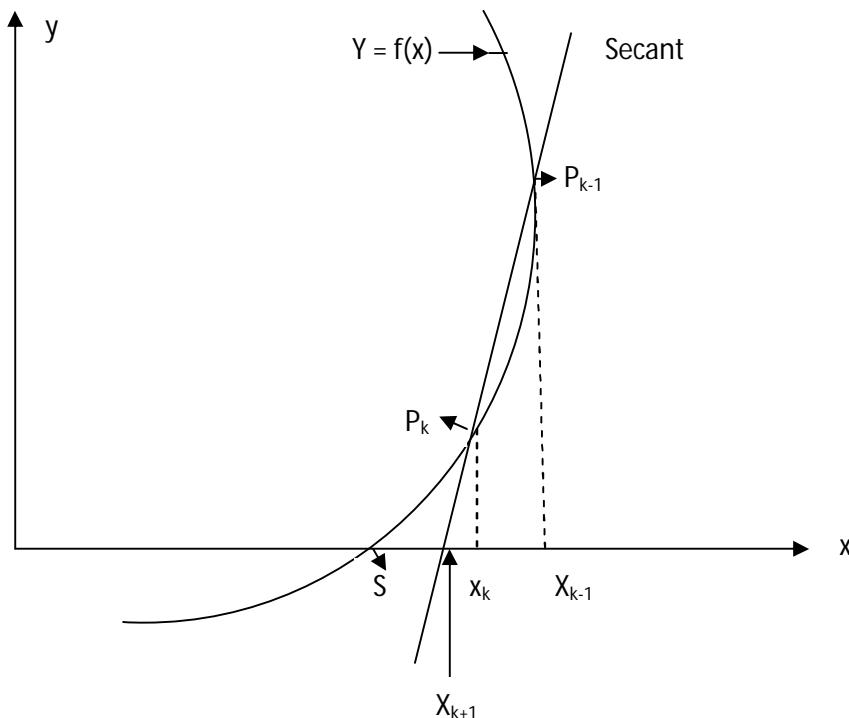
We obtain the Secant method from the Newton-Raphson method, replacing the derivative $F'(x)$ by the difference quotient:

$$f'(x_k) = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Then instead of using $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$ (as in Newton-Raphson's), we have

$$x_{k+1} = x_k - f(x_k) \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})}$$

Geometrically, we intersect the x-axis at x_{k+1} with the secant of $f(x)$ passing through P_{k-1} and P_k in the figure below.



We thus, need two starting values x_0 and x_1 .

CHAPTER THREE

COMPUTATION OF SOME STANDARD FUNCTIONS

Consider the sine x series:

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots$$

For a given value of x , $\sin x$ can be evaluated by summing up the terms of the right hand side. Similarly, $\cos x$, e^x , etc can also be found from the following series;

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \dots$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$$

Example:

Solve $\sin(0.25)$ correct to five decimal places.

Solution;

Given that $x = 0.25$

$$\frac{x^3}{3!} = \frac{x^3}{6} = \frac{(0.25)^3}{6} = 0.0026041$$

$$\frac{x^5}{5!} = \frac{x^5}{120} = \frac{(0.25)^5}{120} = 0.0000081$$

$$\frac{x^7}{7!} = \frac{x^7}{5040} = \frac{(0.25)^7}{5040} = 0.0000000$$

(correct to 6 D)

Therefore,

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} = 0.25 - 0.002641 + 0.0000081$$

$$= 0.2475071 = 0.24751 \text{ (correct to 5D) in radians}$$

1. Taylor's Series Expansion

Let $F(x)$ be a function. We want to write $f(x)$ as a power series about a point x_0 . That is, we want to write $f(x)$ as:

$$f(x) = c_0 + c_1(x - x_0) + c_2(x - x_0)^2 + \dots \dots \dots \quad (1)$$

Where c_0, c_1, c_2, \dots , are constants.

We are interested in finding the constants c_0, c_1, \dots , given $f(x)$ and x_0 .

Therefore, from equation (1),

$$c_0 = f(x_0)$$

If we differentiate equation (1), we obtain:

$$c_1 + 2c_2(x - x_0) + 3c_3(x - x_0)^2 + \dots \dots \dots \quad (2)$$

Therefore,

$$f'(x_0) = c_1 \text{ or } c_1 = f'(x_0)$$

Differentiating equation (2), we obtain:

$$f''(x_0) = 2c_2 + 3(2)(c_3)(x - x_0)$$

Hence,

$$f''(x_0) = 2c_2 \text{ or } c_2 = \frac{f''(x_0)}{2!}$$

Proceeding like this, we shall get;

$$c_3 = \frac{f'''(x_0)}{3!} \text{ and } c_4 = \frac{f^{(iv)}(x_0)}{4!}$$

In general,

$$c_k = \frac{f^{(k)}(x_0)}{k!}$$

Equation (1) thus becomes;

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \dots \dots \dots \quad (3)$$

This is called the Taylor's series expansion about x_0 .

Taylor's series can be expressed in various forms. Putting $x = x_0 + h$ in equation (3), we get another form of Taylor's series:

$$f(x_0 + h) = f(x_0) + \frac{f'(x_0)}{1!} h + \frac{f''(x_0)}{2!} h^2 + \dots \dots \dots \text{-----} \quad (4)$$

Some authors use x in the place of h in equation (4), so we get yet another form of Taylor's series;

$$f(x_0 + x) = f(x_0) + \frac{f'(x_0)}{1!} x + \frac{f''(x_0)}{2!} x^2 + \dots \dots \dots \text{-----} \quad (5)$$

2. The Maclaurin's Series

The Taylor's series of equation (5) about $x_0 = 0$ is called Maclaurin's series of $f(x)$, that is,

$$f(x) = f(0) + \frac{f'(0)}{1!} x + \frac{f''(0)}{2!} x^2 + \dots \dots \dots \text{-----} \quad (6)$$

3. Binomial Series

Consider,

$$f(x) = (1 + x)^n$$

$$f'(x) = n(1 + x)^{n-1}$$

$$f''(x) = n(n - 1)(1 + x)^{n-2}$$

$$f'''(x) = n(n - 1)(n - 2)(1 + x)^{n-3}$$

Now applying the above to the Maclaurin's series, we obtain, noting that;

$$f(0) = 1$$

$$f'(0) = n$$

$$f''(0) = n(n - 1)$$

$$f'''(0) = n(n - 1)(n - 2)$$

So we obtain:

$$(1 + x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3$$

This is the Binomial series.

Example

Derive the Maclaurin's series for e^{-x} and hence, evaluate $e^{-0.2}$ correct to two decimal places.

Solution:

$$f(x) = e^{-x}, \quad f(0) = 1$$

$$f'(x) = -e^{-x}, \quad f'(0) = -1$$

$$f''(x) = e^{-x}, \quad f''(0) = 1$$

$$f'''(x) = -e^{-x}, \quad f'''(0) = -1$$

Now, by Maclaurin's series,

$$f(x) = f(0) + \frac{f'(0)}{1!}x + \frac{f''(0)}{2!}x^2 + \dots \dots \dots$$

That is,

$$e^{-x} = 1 - \frac{x}{1!} + \frac{x^2}{2!} - \frac{x^3}{3!} + \dots \dots \dots$$

Therefore,

$$\begin{aligned} e^{-0.2} &= 1 - 0.2 + \frac{(0.2)^2}{2} - \frac{(0.2)^3}{6} + \frac{(0.2)^4}{24} - \dots \\ &= 0.81 \text{ (to 2D).} \end{aligned}$$

CHAPTER FOUR

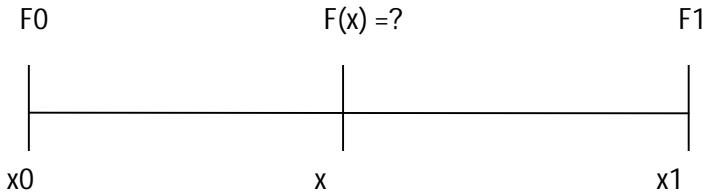
INTERPOLATION

Suppose $F(x)$ is a function whose value at certain points x_0, x_1, \dots, x_n are known. The values are $f(x_0), f(x_1), \dots, f(x_n)$. Consider a point x different from x_0, x_1, \dots, x_n . $F(x)$ is not known.

We can find an approximate value of $F(x)$ from the known values. This method of finding $F(x)$ from these known values is called interpolation. We say that we interpolate $F(x)$ from $f(x_0), f(x_1), \dots, f(x_n)$.

Linear Interpolation

Let x_0, x_1 be two points and f_0, f_1 be the function values at these two points respectively. Let x be a point between x_0 and x_1 . We are interested in interpolating $F(x)$ from the values $F(x_0)$ and $F(x_1)$.



Now consider the Taylor's series:

$$f(x_1) = f(x_0) + \frac{f'(x_0)}{1!}(x_1 - x_0) + \dots \dots \dots$$

Considering only the first two terms, we have:

$$f_1 = f_0 + f'(x_0)(x_1 - x_0)$$

Therefore,

$$f'(x_0) = \frac{f_1 - f_0}{x_1 - x_0}$$

The Taylor's series at x gives

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x - x_0) + \dots \dots \dots$$

Also considering the first the first two terms, we have:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) = f_0 + \frac{(f_1 - f_0)}{(x_1 - x_0)}(x - x_0)$$

Now let $\frac{x-x_0}{x_1-x_0}$ be denoted by p

$$\text{We thus get; } f(x) = f_0 + (f_1 - f_0)p = f_0 + pf_1 - pf_0 = f_0 - pf_0 + pf_1$$

Therefore,

$$f(x) = (1 - p)f_0 + pf_1$$

This is called the linear interpolation formula. Since x is a point between x_0 and x_1 , p is a non-negative fractional value, i.e. $0 \leq p \leq 1$

Example

Consider the following table:

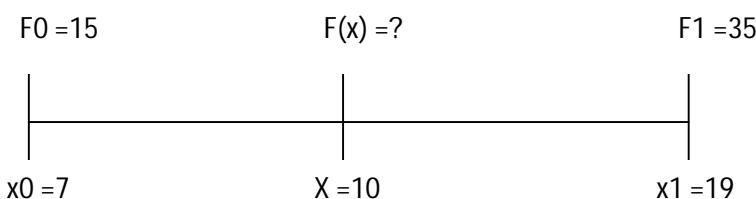
x_i	7	19
f_i	15	35

Find the value of $f(10)$

Solution:

$$x_0 = 7, \quad x_1 = 19$$

$$f_0 = 15, \quad f_1 = 35$$



$$p = \frac{x - x_0}{x_1 - x_0} = \frac{10 - 7}{19 - 7} = \frac{3}{12}$$

$$= 0.25$$

Therefore,

$$1 - p = 1 - 0.25 = 0.75$$

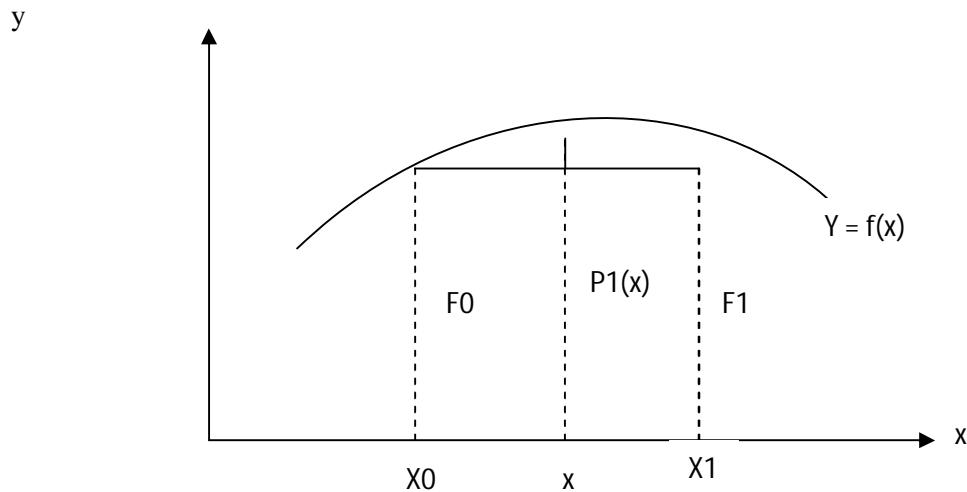
$$\text{Hence, } f(x) = (1 - p)f_0 + pf_1$$

$$= (0.75 \times 15) + (0.25 \times 35) = 11.25 + 8.75$$

$$F(10) = 20$$

Lagrange Interpolation

Linear Lagrange interpolation is interpolation by the straight line through (x_0, f_0) , (x_1, f_1)



Thus, by that idea, the linear Lagrange polynomial P_1 is the sum $P_1 = L_0 f_0 + L_1 f_1$ with L_0 , the linear polynomial that is 1 at x_0 and 0 at x_1 .

Similarly, L_1 is 0 at x_0 and 1 at x_1 .

Therefore,

$$L_0(x) = \frac{x - x_1}{x_0 - x_1}, L_1(x) = \frac{x - x_0}{x_1 - x_0}$$

This gives the linear Lagrange polynomial;

$$P_1(x) = L_0 f_0 + L_1 f_1 = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1$$

Example 1

Compute $\ln 5.3$ from $\ln 5.0 = 1.6094$, $\ln 5.7 = 1.7405$ by linear Lagrange interpolation and determine the error from $\ln 5.3 = 1.6677$.

Solution;

$$x_0 = 5.0$$

$$x_1 = 5.7$$

$$f_0 = \ln 5.0$$

$$f_1 = \ln 5.7$$

Therefore.

$$L_0(5.3) = \frac{5.3 - 5.7}{5.0 - 5.7} = \frac{-0.4}{-0.7} = 0.57$$

$$L_1(5.3) = \frac{5.3 - 5.0}{5.7 - 5.0} = \frac{0.3}{0.7} = 0.43$$

Hence,

$$\begin{aligned} \ln 5.3 &= L_0(5.3)f_0 + L_1(5.3)f_1 \\ &= 0.57 \times 1.6094 + 0.43 \times 1.7405 = 1.6658 \end{aligned}$$

The error is $1.6677 - 1.6658 = 0.0019$

The quadratic Lagrange Interpolation

This interpolation of given $(x_0, f_0), (x_1, f_1), (x_2, f_2)$ by a second degree polynomial $P_2(x)$, which by Lagrange's idea, is:

$$P_2(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2$$

With,

$$L_0(x_0) = 1, L_1(x_1) = 1, L_2(x_2) = 1 \text{ and}$$

$L_0(x_1) = L_0(x_2) = 0$, e.t.c., we therefore claim that:

$$L_0(x) = \frac{l_0(x)}{l_0(x_0)} = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$L_1(x) = \frac{l_1(x)}{l_1(x_1)} = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$L_2(x) = \frac{l_2(x)}{l_2(x_2)} = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

The above relations are valid since, the numerator makes $L_k(x_j) = 0$ if $j \neq k$; and the denominator makes $L_k(x_k) = 1$ because it equals the numerator at $x = x_k$

Example 2

Compute $\ln 5.3$ by using the quadratic Lagrange interpolation, using the data of example 1 and $\ln 7.2 = 1.9741$. Compute the error and compare the accuracy with the linear Lagrange case.

Solution:

$$L_0(5.3) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \frac{(5.3 - 5.7)(5.3 - 7.2)}{(5.0 - 5.7)(5.0 - 7.2)}$$

$$= \frac{(-0.4)(-1.9)}{(-0.7)(-2.2)} = \frac{0.76}{1.54} = 0.4935$$

$$L_1(5.3) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} = \frac{(5.3 - 5.0)(5.3 - 7.2)}{(5.7 - 5.0)(5.7 - 7.2)}$$

$$= \frac{(0.3)(-1.9)}{(0.7)(-1.5)} = \frac{-0.57}{-1.05} = 0.5429$$

$$\begin{aligned} L_2(5.3) &= \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} = \frac{(5.3 - 5.0)(5.3 - 5.7)}{(7.2 - 5.0)(7.2 - 5.7)} \\ &= \frac{(0.3)(-0.4)}{(2.2)(1.5)} = \frac{-0.12}{3.3} = -0.03636 \end{aligned}$$

Therefore,

$$\begin{aligned} \ln 5.3 &= L_0(5.3)f_0 + L_1(5.3)f_1 + L_2(5.3)f_2 \\ &= 0.4935 \times 1.6094 + 0.5429 \times 1.7405 + (-0.03636) \times 1.9741 \\ &= 0.7942 + 0.9449 - 0.07177 = 1.6673 \text{ (4D)} \end{aligned}$$

The error = 1.6677 - 1.6673 = 0.0004

The above results show that the Lagrange quadratic interpolation is more accurate for this case.

Generally, the Lagrange interpolation polynomial may be written as:

$$f(x) \cong P_n(x) = \sum_{k=0}^n L_k(x)f_k = \sum_{k=0}^n \frac{l_k(x)}{l_k(x_k)} f_k$$

Where,

$$L_k(x_k) = 1 \text{ and } 0 \text{ at the other nodes}$$

CHAPTER FIVE

INTRODUCTION TO FINITE DIFFERENCES

Consider a function: $f(x) = x^3 - 5x^2 + 6$

The table below illustrates various finite difference parameters.

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f \dots\dots\dots$
0	6				
1	2	- 4			
2	-6	- 8	- 4	6	
3	-12	- 6	2	6	
4	-10	2	8	6	
5	6	16	14	6	
6	42	36	20		

Notice that a constant (6) occurs in the forward difference at $\Delta^3 f$ (3rd forward difference)

It can be shown that:

$$\Delta^3 f = \frac{d^3 f}{dx^3}$$

Therefore,

$$\frac{d^3 f}{dx^3} = 6$$

$$\frac{d^2 f}{dx^2} = 6x + A$$

$$\frac{dy}{dx} = 3x^2 + Ax + B$$

Hence, $f = x^3 + \frac{A}{2}x^2 + Bx + C$

We now determine the constants:

$$\text{At } x = 0, f(x) = 6 = C$$

$$\text{Therefore, } f(x) = x^3 + \frac{A}{2}x^2 + Bx + 6$$

At $x = 1, f(x) = 2$ (from the table)

$$\text{Therefore, } 2 = 1 + \frac{A}{2} + B + 6, \quad \dots \quad (1)$$

$$\text{At } x = 2, f(x) = -6$$

Hence,

$$-6 = 8 + \frac{A}{2}(4) + 2B + 6 \quad \text{-----} \quad (2)$$

We then solve simultaneously for the other constants.

The first forward difference is generally taken as an approximation for the first difference, i.e. $\Delta f \cong f'(x)$, (but will be exact if linear). Also, $\Delta^2 f \cong f''(x)$ (but exact if quadratic).

Similarly, $\Delta^3 f \cong f'''(x)$ (but exact if cubic).

Note also that;

$f(x)$ will be linear if the constant terms occur at Δf column, quadratic if they occur at $\Delta^2 f$ column and cubic if at $\Delta^3 f$ column.

Now,

$$\Delta f \cong f'(x) = \frac{f_1 - f_0}{x_1 - x_0} = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

Let $x_{i+1} - x_i = h$ = interval,

Then,

$$f'(x) = \frac{f_{i+1} - f_i}{h}$$

Now, from the Taylor's series expansion, let us on this occasion consider the expansion about a point x_i :

$$f_{i+1} = f_i + hf_i^{(1)} + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i^{(3)} + \dots \dots \dots \quad (1)$$

In this and subsequently, we denote the nth derivative evaluated at x_i by $f_i^{(n)}$

Hence,

$$f_{i-1} = f_i - hf_i^{(1)} + \frac{h^2}{2!}f_i^{(2)} - \frac{h^3}{3!}f_i^{(3)} + \dots \dots \dots \quad (2)$$

From equations one and two, three different expressions that approximate $f_i^{(1)}$ can be derived.

The first is from equation (1), considering the first two terms:

$$f_{i+1} - f_i = hf_i^{(1)} + \frac{h^2}{2!}f_i^{(2)}$$

Therefore, $\frac{f_{i+1} - f_i}{h} = f_i + \frac{h}{2!}f_i^{(2)}$

Hence, $f_i^{(1)} \equiv \left(\frac{df}{dx}\right)_{x_i} = \frac{f_{i+1} - f_i}{h} - \frac{h}{2!}f_i^{(2)} \quad (3)$

The quantity $\frac{f_{i+1} - f_i}{h}$ is known as the forward difference and it is clearly a poor approximation, since it is in error by approximately $\frac{h}{2}f_i^{(2)}$.

The second of the expressions is from equation (2), considering the first two terms:

$$f_i - f_{i-1} = hf_i^{(1)} - \frac{h^2}{2!}f_i^{(2)}$$

Therefore, $\frac{f_i - f_{i-1}}{h} = f_i^{(1)} - \frac{h^2}{2!}f_i^{(2)}$

Hence, $f_i^{(1)} \equiv \left(\frac{df}{dx}\right)_{x_i} = \frac{f_i - f_{i-1}}{h} + \frac{h^2}{2!}f_i^{(2)} \quad (4)$

Also, the quantity $\frac{f_i - f_{i-1}}{h}$ is called the backward difference. The sign of the error is reversed, compared to that of the forward difference.

The third expression is obtained by subtracting equation (2) from equation (1), we then have:

$$\begin{aligned} f_{i+1} - f_{i-1} &= hf_i^{(1)} + hf_i^{(1)} + 2 \frac{h^3}{3!} f_i^{(3)} \\ &= 2hf_i^{(1)} + 2h^3 \frac{f_i^{(3)}}{3!} \end{aligned}$$

Hence,

$$f_{i+1} - f_{i-1} = 2h \left(f_i^{(1)} + \frac{h^2 f_i^{(3)}}{3!} \right)$$

Therefore,

$$\frac{f_{i+1} - f_{i-1}}{2h} = f_i^{(1)} + \frac{h^2 f_i^{(3)}}{3!}$$

So,

$$f_i^{(1)} \equiv \left(\frac{df}{dx} \right)_{x_i} = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2 f_i^{(3)}}{3!} \quad (5)$$

The quantity, $\frac{f_{i+1} - f_{i-1}}{2h}$ is known as the central difference approximation to $f_i^{(1)}$ and can be seen from equation (5) to be in error by approximately $\frac{h^2}{6} f_i^{(3)}$. Note that this is a better approximation compared to either the forward or backward difference.

By a similar procedure, a central difference approximation to $f_i^{(2)}$ can be obtained:

$$f_i^{(2)} = \left(\frac{d^2 f}{dx^2} \right)_{x_i} \cong \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \quad (6)$$

The error in this approximation, also known as the second difference of f , is about $\frac{h^2}{12}$ (4)

It is obvious that the second difference approximation is far better than the first difference.

Example:

The following is copied from the tabulation of a second degree polynomial $f(x)$ at values of x from 1 to 12 inclusive.

2, 2, ?, 8, 14, 22, 32, 46, ?, 74, 92, 112

The entries marked ? were illegible and in addition, one error was made in transcription.

Complete and correct the table.

Solution:

S/N	$f(x)$	Δf	$\Delta^2 f$	
1	2			Because, the polynomial is second degree, the 2 nd
2	2	0	?	differences (which are proportional to $\frac{d^2 f}{dx^2}$) should be
3	?	?	?	constant and clearly, this should be 2. Hence, the 6 th value in
4	8	?	?	the $\Delta^2 f$ column should be 2 and also all the ? in this column.
5	14	6	2	Equally, the 7 th value in the Δf column should be 12 and not
6	22	8	2	14. And since all the values in the $\Delta^2 f$ column are a constant
7	32	10	4	, 2, the first two ? in Δf column are 2 and 4 respectively and
8	46	14	?	the last two are 14 and 16 respectively. Working this
9	?	?	?	backward to $f(x)$ column, the first ? = 4, while the 8 th value
10	74	18	?	in this column = 44 and not 46.. Finally, the last ? in the
11	92	20	2	$f(x)$ column = 58
12	112			The entries should therefore read: 2, 2, 4, 8, 14, 22, 32, 44, 58, 74, 92, 112

CHAPTER SIX

SIMULTANEOUS LINEAR EQUATIONS

Consider a set of N simultaneous linear equations in N variables (unknowns), $x_i, i = 1, 2, \dots, N$.

The equations take the general form:

$$A_{11}x_1 + A_{12}x_2 + \dots + A_{1N}x_N = b_1$$

$$A_{21}x_1 + A_{22}x_2 + \dots + A_{2N}x_N = b_2$$

----- (1)

$$A_{N1}x_1 + A_{N2}x_2 + \dots + A_{NN}x_N = b_N$$

Where, A_{ij} are constants and form the elements of a square matrix A. The b_i are given and form a column vector b . If A is non-singular, equation (1) can be solved for the x_i using the inverse of A according to the formula; $x = A^{-1}b$.

Systems of linear Equations

Consider the following system of linear equations:

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = a_{1,n+1}$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = a_{2,n+1}$$

$$a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n = a_{n,n+1}$$

A solution to this system of equations is a set of values x_1, x_2, \dots, x_n which satisfies the above equations.

Consider the matrix:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \dots \dots a_{1n} \\ a_{21} & a_{22} & a_{23} \dots \dots a_{2n} \\ a_{n1} & a_{n2} & a_{n3} \dots \dots a_{nn} \end{bmatrix}$$

This called the coefficient matrix

The vector: $\begin{bmatrix} a_{1,n+1} \\ \vdots \\ a_{n,n+1} \end{bmatrix}$ is called the right hand side vector.

In some special cases, the solution can be got directly.

Cases 1

A square matrix is called a diagonal matrix if the diagonal entries alone are non-zeros. Suppose the coefficient matrix is a diagonal matrix, i.e. the coefficient matrix is of the form:

$$\begin{bmatrix} a_{11} & 0 & 0 \dots \dots 0 \\ 0 & a_{22} & 0 \dots 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \dots a_{nn} \end{bmatrix}$$

The equations will be of the form:

$$a_{11}x_1 = a_{1,n+1}$$

$$a_{22}x_2 = a_{2,n+1}$$

— — — — —

— — — — —

$$a_{nn}x_n = a_{n,n+1}$$

In this case, the solution can be directly written as:

$$x_1 = \frac{a_{1,n+1}}{a_{11}}, \quad x_2 = \frac{a_{2,n+1}}{a_{22}}, \dots \dots \dots, \quad x_n = \frac{a_{n,n+1}}{a_{nn}}$$

Case 2

A matrix is said to be lower triangular if all its upper diagonal entries are zeros.

Suppose the coefficient matrix is a lower diagonal matrix, i.e. it is of the following form:

$$\begin{bmatrix} a_{11} & 0 & 0 \dots 0 \\ a_{21}a_{22} & 0 \dots 0 \\ \hline \hline a_{n1}a_{n2}a_{n3} \dots a_{nn} \end{bmatrix}$$

The equations will be of the following form:

$$a_{11}x_1 = a_{1,n+1}$$

$$a_{21}x_1 + a_{22}x_2 = a_{2,n+1}$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = a_{3,n+1}$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n = a_{n,n+1}$$

From the first equation,

$$x_1 = \frac{a_{1,n+1}}{a_{11}}$$

Substituting x_1 into the second equation, we have:

$$x_2 = \frac{1}{a_{22}}(a_{2,n+1} - a_{21}x_1)$$

Also, doing the same for x_2 :

$$x_3 = \frac{1}{a_{33}}(a_{3,n+1} - a_{31}x_1 - a_{32}x_2)$$

Similarly, we can find x_4, x_5, \dots, x_n . This is called forward substitution method.

Case 3

Suppose the coefficient is upper triangular. Then, the equations will be of the following form;

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = a_{1,n+1}$$

$$0 + a_{22}x_2 + \dots + a_{2n}x_n = a_{2,n+1}$$

$$+ a_{nn}x_n = a_{n,n+1}$$

Starting from the last equation,

$$x_n = \frac{a_{n,n+1}}{a_{nn}}$$

The $(n - 1)$ th equation can now be used to evaluate x_{n-1} thus:

$$x_{n-1} = \frac{1}{a_{n-1,n-1}}(a_{n-1,n-1} - a_{n-1,n}x_n)$$

In general, after evaluating $x_n, x_{n-1}, \dots, x_{k+1}$, we evaluate x_k as:

$$x_k = \frac{1}{a_{kk}} = (a_{k,n+1} - a_{k,k+1}x_{k+1} - \dots - a_{kn}x_n)$$

We can thus evaluate all the x_i values. This is called backward substitution method.

Elementary Row Operations

Consider a matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \hline \hline & & & & \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix}$$

Operation 1

Multiplying each element of a row by a constant:

If the i th row is multiplied by a constant k , we write: $R_i = kR_i$ (read as R_i becomes kR_i).

Operation 2

Multiplying one row by a constant and subtracting it from another row, i.e. R_i can be replaced by $R_i - kR_j$. We write $R_i \leftarrow R_i - kR_j$.

Operation 3

Two rows can be exchanged: If R_i and R_j are exchanged, we write $R_i \leftrightarrow R_j$.

When operation 1 is performed, the determinant is multiplied by k .

If operation 2 is performed on a matrix, its determinant value is not affected.

When operation 3 is performed, the sign of its determinant value reverses.

Now consider a matrix in which all the lower diagonal entries of the first column are zero;

$$A = \begin{matrix} a_{11} & a_{12} & a_{13} \dots a_{1n} \\ 0 & a_{22} & a_{23} \dots a_{2n} \\ 0 & a_{32} & a_{33} \dots a_{3n} \\ \dots & & \\ 0 & a_{n2} & a_{n3} \dots a_{nn} \end{matrix}$$

$$|A| = a_{11} \begin{bmatrix} a_{22} & a_{23} \dots & a_{2n} \\ a_{32} & a_{33} \dots & a_{3n} \\ a_{n2} & a_{n3} \dots & a_{nn} \end{bmatrix}$$

Pivotal Condensation

Consider a matrix,

$$A = \begin{matrix} a_{11} & a_{12} & a_{13} \dots a_{1n} \\ a_{21} & a_{22} & a_{23} \dots a_{2n} \\ \dots & \dots & \dots \\ a_{n1} & a_{n2} & a_{n3} \dots a_{nn} \end{matrix}$$

Also consider a row operation $R \leftarrow R_2 - \frac{a_{21}}{a_{11}} R_1$, performed on the matrix A; then the

a_{21} entry will become zero. Similarly, do the operation $R_i \leftarrow R_i - \frac{a_{i1}}{a_{11}} R_1$, for $i = 2, 3, 4, \dots, n$

Then the lower diagonal entries of the first column will become zero. Note that these operations not affect the determinant value of A.

In the above operation, a_{ij} would have now become:

$$a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}, \text{ that is: } a_{ij} \leftarrow a_{ij} - \frac{a_{i1}}{a_{11}} a_{1j}$$

Therefore, according to the new notation:

$$\begin{matrix} a_{11} & a_{12} & a_{13} \dots a_{1n} \\ A = 0 & a_{22} & a_{23} \dots a_{2n} \\ 0 & a_{32} & a_{33} \dots a_{3n} \\ \dots\dots\dots \\ 0 & a_{n2} & a_{n3} \dots a_{nn} \end{matrix}$$

$$|A| = a_{11} \begin{bmatrix} a_{22} & a_{23} \dots & a_{2n} \\ a_{32} & a_{33} \dots & a_{3n} \\ a_{n2} & a_{n3} \dots & a_{nn} \end{bmatrix}$$

Now, we can once again repeat the above procedure on the reduced matrix to get determinant:

$$|A| = a_{11} a_{22} \begin{bmatrix} a_{33} a_{34} & \dots & a_{3n} \\ \vdots & \ddots & \vdots \\ a_{n3} a_{n4} & \dots & a_{nn} \end{bmatrix}$$

‘A’ was a $n \times n$ matrix. In the first step, we condensed it into a $(n - 1) \times (n - 1)$ matrix. Now, it has further been condensed into $(n - 2) \times (n - 2)$ matrix. Repeating the above procedure, we can condense the matrix into 1×1 . So, determinant, $A = a_{11} \cdot a_{22} \cdot a_{33} \dots a_{nn}$.

Algorithm Development

Let A be the given matrix,

1. Do the row operation $R_i \leftarrow R_i - \frac{a_{i1}}{a_{11}} R_1$

(for $i = 2, 3, 4, \dots, n$)

This makes all the lower diagonal entries of the first column zero.

2. Do the row operation $R_i \leftarrow R_i - \frac{a_{i2}}{a_{22}} R_2$ (for $i = 3, 4, \dots, n$)

This also makes all the lower diagonal entries of the second column zero.

3. Do the row operation $R_i \leftarrow R_i - \frac{a_{i3}}{a_{33}} R_3$ (for $i = 4, 5, \dots, n$)

This makes all the lower diagonal entries of the third column zero.

In general, in order to make the lower diagonal entries of the k^{th} column zero,

4. Do the row operation, $R_i \leftarrow R_i - \frac{a_{ik}}{a_{kk}} R_k$ for $i = k + 1, k + 2, \dots, n$)

Doing the above operation for $k = 1, 2, 3, \dots, n - 1$, makes all the lower diagonal entries of the matrix zero. Hence, determinant $A = a_{11} \cdot a_{22} \cdot a_{33} \cdots a_{nn}$.

Notice that the following segment will do the required row operation:

$$ratio = \frac{a_{ik}}{a_{kk}}$$

For $j = 1$ to n

$$a_{ij} = a_{ij} - ratio * a_{kj}$$

next j

This operation has to be repeated for $i = k + 1$ to n in order to make the lower diagonal entries of the k^{th} column zero.

The complete algorithm is show below:

1. Read n
2. *for* $i = 1$ to n
3. *for* $j = 1$ to n
4. *Read* a_{ij}
5. *next j*
6. *next i*
7. *for* $k = 1$ to $n - 1$
8. *for* $i = k + 1$ to n

9. $ratio = \frac{a_{ik}}{a_{kk}}$
10. *for* $j = 1$ to n
11. $a_{ij} = a_{ij} - ratio * a_{kj}$
12. *next j*
13. *next i*
14. *next k*
15. $Det = 1$
16. *for* $i = 1$ to n
17. $Det = Det * a_{ii}$
18. *next i*
19. *Print Det*
20. *End.*

Practice Questions

1. Write a FORTRAN program to implement the pivotal condensation method, to find the determinant of any matrix of order n .
2. Find the determinant of :

$$\begin{array}{cccc} & 1.2 & -2.1 & 3.2 & 4.3 \\ -1.4 & -2.6 & 3.0 & 4.1 & \\ & -2.2 & 1.7 & 4.0 & 1.2 \\ & 1.1 & 3.6 & 5.0 & 4.6 \end{array}$$

Using the pivotal condensation method,

Gauss Elimination Method

Consider the equation:

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = a_{1,n+1}$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = a_{2,n+1}$$

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = a_{n,n+1}$$

This can be in matrix form and solved using the row operation which was done for the pivotal condensation method.

The algorithm consists of three major steps thus:

- (i) Read the matrix
- (ii) Reduce it to upper triangular form
- (iii) Use backward substitution to get the solution..

Algorithm:

Read Matrix A.

1. Read n
2. *for* $i = 1$ to n
3. *for* $j = 1$ to $n + 1$
4. Read a_{ij}
5. Next j
6. Next i

Reduce to upper Triangular

7. *for* $k = 1$ to $n - 1$
8. *for* $i = k + 1$ to n
9. $Ratio = \frac{a_{ik}}{a_{kk}}$

10. *for* $j = 1$ to $n + 1$
11. $a_{ij} = a_{ij} - Ratio * a_{kj}$
12. Next j
13. Next i
14. Next k

Backward Substitution

15. $x_n = \frac{a_{n,n+1}}{a_{nn}}$
16. *for* $k = n - 1$ to 1 step -1
17. $x_k = a_{k,n+1}$
18. *for* $j = k + 1$ to n
19. $x_k = x_k - a_{kj} * x_j$
20. Next j
21. $x_k = \frac{x_k}{a_{kk}}$
22. Next k

Print Answer

23. *for* $i = 1$ to n
24. *print* x_i
25. Next i
26. End

Example:

Solve the following system of equations by the Gauss elimination method:

$$x_1 + x_2 + \frac{1}{2}x_3 + x_4 = 3.5$$

$$-x_1 + 2x_2 + x_4 = -2$$

$$-3x_1 + x_2 + 2x_3 + x_4 = -3$$

$$-x_1 + 2x_4 = 0$$

Solution: The matrix is:

$$\begin{array}{cccccc}
 1 & 1 & 0.5 & 1 & 3.5 \\
 -1 & 2 & 0 & 1 & -2 \\
 -3 & 1 & 2 & 1 & -3 \\
 -1 & 0 & 0 & 2 & 0
 \end{array}$$

In order to make zero, the lower diagonal entries of the first column, do the following operations

$$R_2 \leftarrow R_2 + R_1$$

$$R_3 \leftarrow R_3 + 3R_1$$

$$R_4 \leftarrow R_4 + R_1$$

These will yield:

$$\begin{array}{cccccc}
 1 & 1 & 0.5 & 1 & 3.5 \\
 0 & 3 & 0.5 & 2 & 1.5 \\
 0 & 4 & 3.5 & 4 & 7.5 \\
 0 & 1 & 0.5 & 3 & 3.5
 \end{array}$$

Now do the operations:

$$R_3 \leftarrow R_3 - \frac{4}{3}R_2$$

$$R_4 \leftarrow R_4 - \frac{R_2}{3}$$

These will yield:

$$\begin{array}{cccccc}
 1 & 1 & 0.5 & 1 & 3.5 \\
 0 & 3 & 0.5 & 2 & 1.5 \\
 0 & 0 & 2.833 & 1.33 & 5.5 \\
 0 & 0 & 0.66 & 2.33 & 3
 \end{array}$$

Now, doing:

$$R_4 \leftarrow R_4 - \frac{0.66}{2.33} * R_3$$

Will result to:

$$\begin{array}{r}
 & 1 & 1 & 0.5 & 1 & 3.5 \\
 0 & 3 & 0.5 & 2 & 1.5 & \\
 & 0 & 0 & 2.833 & 1.33 & 5.5 \\
 & 0 & 0 & 0 & 2.0196 & 1.70588
 \end{array}$$

Now the equations become:

$$x_1 + x_2 + \frac{1}{2}x_3 + x_4 = 3.5 \quad \dots \quad (1)$$

$$3x_2 + \frac{1}{2}x_3 + 2x_4 = 1.5 \quad \dots \quad (2)$$

$$2.833x_3 + 1.33x_4 = 5.5 \quad \dots \quad (3)$$

$$2.0196x_4 = 1.70588 \quad \dots \quad (4)$$

From equation (4),

$$x_4 = 0.84466$$

From equation (3),

$$2.833x_3 + 1.33(0.84466) = 5.5$$

$$\rightarrow x_3 = 1.544$$

Also, from equation (2),

$$3x_2 + \frac{1}{2}(1.544) + 2(0.84466) = 1.5$$

$$\rightarrow x_2 = -0.3204$$

Finally, equation (1) gives, after substituting x_4, x_3 , and x_2 values:

$$x_1 = 2.2039$$

CHAPTER SEVEN

DIFFERENTIAL EQUATIONS

The following are some differential equations:

$$y' = (x^2 + y)e^x$$

$$y'' = y'x + xy^2$$

$$xy''' + (1 - x^2)yy'' + y = (x^2 - 1)e^u$$

If $y^{(k)}$ is the highest order derivative in a differential equation, the equation is said to be a k^{th} order differential equation.

A solution to the differential equation is the value of y which satisfies the differential equation.

Example:

Consider the differential equation: $y'' = 6x + 4$

This is a second order differential equation. The function:

$$y = x^3 + 2x^2 - 1$$

satisfies the differential equation, hence, $y = x^3 + 2x^2 - 1$ is a solution to the differential equation.

Numerical Solutions

Consider the equation: $y'' = 6x + 4$

A solution is $y = x^3 + 2x^2 - 1$, however, instead of writing the solution as a function of x , we can find the numerical values of y for various pivotal values of x . The solution from $x = 0$ to $x = 1$ can be expressed as follows:

x	0	0.2	0.4	0.6	0.8	1.0
y	-1	-0.912	-0.616	0.064	0.792	2.0

The values are got by the function $y = x^3 + 2x^2 - 1$. This table of numerical values of y is said to be a numerical solution to the differential equation.

The initial value Problem

Consider the differential equation: $y' = f(x, y); y(x_0) = y_0$

This is a first order differential equation. Here, the y value at $x_0 = y_0$. The solution y at x_0 is given, We must assume a small increment h . i.e.

$$x_1 = x_0 + h$$

$$x_2 = x_1 + h$$

— — —

$$x_{i+1} = x_i + h$$

y_0	$y_1 = ?$	$y_2 = ?$	$y_3 = ?$	$y_4 = ?$
x_0	x_1	x_2	x_3	x_4

Let us denote the y values at x_1, x_2, \dots as y_1, y_2, \dots respectively. y_0 is given and so we must find y_1, y_2, \dots . This differential equation is called an initial value problem.

Euler's Method

Consider the initial value problem: $y' = f(x, y); y(x_0) = y_0$

y is a function of x, so we shall write that function as $y(x)$

Using the Taylor's series expansion:

$$y(x_0 + h) = y(x_0) + \frac{h}{1!} y'(x_0) + \frac{h^2}{2!} y''(x_0) + \dots$$

Here, $y(x_0 + h)$ denotes y value at $x_0 + h$

$y'(x_0)$ denotes y' value at $x_0 + h$, e.t.c.

Given;

$$y(x_0) = y_0$$

$$y(x_0 + h) = y(x_1) = y_1 \text{ (say)}$$

$$y'(x_0) = y' \text{ at } x_0$$

But, $y' = f(x, y)$

$$\rightarrow y'(x_0) = f(x_0, y_0)$$

Now, let

$$y'(x_0) = f(x_0, y_0) = f_0$$

$$\text{hence, } y'(x_0) = f_0$$

Therefore, Taylor's series expansion up to the first order term, gives:

$$y_1 = y_0 + hf_0$$

Similarly, we can derive:

$$y_2 = y_1 + hf_1$$

$$y_3 = y_2 + hf_2$$

In general,

$$y_{i+1} = y_i + hf_i, \text{ where } f_i = f(x_i, y_i)$$

This is called the Euler's formula to solve an initial value problem.

Algorithm for Euler's method

1. Define $f(x, y)$
2. Read x_0, y_0, n, h
3. for $i = 0$ to $n - 1$ Do
4. $x_{i+1} = x_i + h$
5. $y_{i+1} = y_i + hf(x_i, y_i)$
6. Print x_{i+1}, y_{i+1}
7. next i
8. End

Assignment: Implement the above in any programming language (FORTRAN or BASIC)

Example:

Solve the initial value problem: $y' = x^2 + y^2; y(1) = 0.8; x = 1(0.5)3$

Solution:

Given: $f(x, y) = x^2 + y^2, x_0 = 1, y_0 = 0.8, h = 0.5, x = 1 \text{ to } 3$

$y_0 = 0.8$	$y_1 = ?$	$y_2 = ?$	$y_3 = ?$	$y_4 = ?$
$x_0 = 1$	$x_1 = 1.5$	$x_2 = 2$	$x_3 = 2.5$	$x_4 = 3$

$$y_1 = y_0 + hf_0$$

$$\text{But } f_0 = f(x_0, y_0) = f(1, 0.8) = 1.64$$

$$\text{Therefore, } y_1 = 0.8 + (0.5)(1.64) = 1.62$$

$$y_2 = y_1 + hf_1$$

$$\text{But } f_1 = f(x_1, y_1) = f(1.5, 1.62) = 4.8744$$

$$\text{Therefore, } y_2 = 1.62 + (0.5)(4.8744) = 4.0572$$

$$y_3 = y_2 + hf_2$$

$$\text{But } f_2 = f(x_2, y_2) = f(2, 4.0572) = 20.460871$$

$$\text{Therefore, } y_3 = 4.0572 + (0.5)(20.460871) = 14.287635$$

$$y_4 = y_3 + hf_3$$

$$\text{But } f_3 = f(x_3, y_3) = f(2.5, 14.287635) = 210.38651$$

$$\text{Therefore, } y_4 = 14.287635 + (0.5)(210.38651) = 119.48088$$

So the numerical solution got by Euler's method is:

$y_0 = 0.8$	$y_1 = 1.62$	$y_2 = 4.0572$	$y_3 = 14.287635$	$y_4 = 119.48088$
$x_0 = 1$	$x_1 = 1.5$	$x_2 = 2$	$x_3 = 2.5$	$x_4 = 3$

Assignment: Using Euler's method, solve: $5 \frac{dy}{dx} = 3x^3y; y(0) = 1$

For the interval $0 \leq x \leq 0.3$, with $h = 0.1$

Backward Euler's Method

The formula for backward Euler's method is given by: $y_{i+1} = y_i + hf_{i+1}$

Where, $f_{i+1} = f(x_{i+1}, y_{i+1})$

For example, consider the initial value problem:

$$y' = 2x^3y; y(0) = 1; x = 0(0.2)0.4$$

Solution:

$$f(x, y) = 2x^3y$$

$$x_0 = 0, y_0 = 1, h = 0.2$$

The backward Euler's method formula is: $y_{i+1} = y_i + hf_{i+1}$

$$\rightarrow y_{i+1} = y_i + h(2x_{i+1}^3 * y_{i+1})$$

Therefore,

$$y_{i+1} - 2hx_{i+1}^3 * y_{i+1} = y_i$$

Hence,

$$y_i = y_{i+1}(1 - 2hx_{i+1}^3)$$

OR

$$y_{i+1} = \frac{y_i}{(1 - 2hx_{i+1}^3)}$$

$y_0 = 1$	$y_1 = ?$	$y_2 = ?$
$x_0 = 0$	$x_1 = 0.2$	$x_2 = 0.4$

Now, put $i = 0$ in the formula:

$$y_1 = \frac{y_0}{(1 - 2hx_1^3)} = \frac{1}{1 - 2(0.2)(0.2)^3} = 1.0032102$$

Put $i = 1$ in the formula:

$$y_2 = \frac{y_1}{(1 - 2hx_2^3)} = \frac{1.0032102}{1 - 2(0.2)(0.4)^3} = 1.0295671$$

Therefore, the numerical solution to the problem is:

$y_0 = 1$	$y_1 = 1.0032102$	$y_2 = 1.0295671$
$x_0 = 0$	$x_1 = 0.2$	$x_2 = 0.4$

Euler-Richardson's Method

The formula is written as

$$y_{i+1} = y_i + \frac{h}{3} \left(f_i + 2f_{i+\frac{1}{2}} \right)$$

Where $f_i = f(x_i, y_i)$ and $f_{i+\frac{1}{2}} = f\left(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}\right)$

Also, $x_{i+\frac{1}{2}} = x_i + \frac{h}{2}$; $y_{i+\frac{1}{2}} = y_i + \frac{h}{2}f_i$

Algorithm

1. Define (f, x)
2. Read x_0, y_0, h, n
3. for $i = 0$ to $n - 1$ Do
4. $x_{i+\frac{1}{2}} = x_i + \frac{h}{2}$
5. $y_{i+\frac{1}{2}} = y_i + \frac{h}{2}f(x_i, y_i)$
6. $x_{i+1} = x_i + h$
7. $y_{i+1} = y_i + \frac{h}{3} \left\{ f(x_i, y_i) + 2f\left(x_{i+\frac{1}{2}}, y_{i+\frac{1}{2}}\right) \right\}$
8. Print x_{i+1}, y_{i+1}
9. Next i
10. End

Let us now, develop a FORTRAN programme for the function: $f(x, y) = \frac{1}{2}(1 + x)y^2$

i.e. $y' = \frac{1}{2}(1 + x)y^2$; $y(0) = 1$; $x = 0(0.1)0.6$

Hence, $x_0 = 0$, $y_0 = 1$, $h = 0.1$, $n = 6$

Note: Let $XM = x_{i+1}$ and $YM = y_{i+1}$

```

C      PROGRAM FOR EULER RICHARDSON

DIMENSION X(20), Y(20)

F(X,Y) = 0.5*(1. +X) *Y*Y

WRITE (*,*) 'ENTER X0 , Y0 , H , N VALUES'

READ (*,5) X(0), Y(0), H, N

5      FORMAT (3F15.5, I5)

WRITE (*,*) X(I), Y(I)

DO 25 I = 0, N-1

XM = X(I) + H/2.0

YM = Y(I) + H/2.0 * F(X(I), Y(I))

X(I+1) = X(I) +H

FI = F(X(I), Y(I))

FM = F(XM, YM)

Y(I+1) = Y(I) +H/3. * (FI + 2.0 * FM)

WRITE (*,15) X(I+1), Y(I+1)

15     FORMAT (1X, 2F15.5)

CONTINUE

STOP

END

```

Taylor's Series Method

Given that y is a function of x , it is written as $y(x)$

By Taylor's series expansion;

$$y(x + h) = y(x) + \frac{y'(x)}{1!}h + \frac{y''(x)}{2!}h^2 + \dots \dots \dots$$

f

$$y(x_i + h) = y_i + \frac{h}{1!}y_i' + \frac{h^2}{2!}y_i'' + \dots \dots \dots$$

Where,

$$y'_i = y' \text{ at } (x_i, y_i)$$

$$y''_i = y'' \text{ at } (x_i, y_i)$$

$$\rightarrow y(x_{i+1}) = y_i + \frac{h}{1!} y'_i + \frac{h^2}{2!} y''_i + \dots \dots \dots$$

Let the given initial value problem to be solved be:

$$y' = f(x, y); \quad y(x_0) = y_0$$

Now consider the problem:

$$y' = 4x^3 + 1$$

$$y(0) = 1.5$$

$$x = 0(0.2)0.8$$

Here,

$$y' = 4x^3 + 1$$

$$y'_i = 4x_i^3 + 1$$

$$y'' = 12x^2 y'_i = 12x_i^2$$

$$y''' = 24xy''_i = 24x_i$$

$$y^{(iv)} = 24y''_i = 24$$

$$y^{(v)} = 0y'_i = 0$$

Therefore, Taylor's expansion becomes:

$$y_{i+1} = y_i + h(4x_i^3 + 1) + \frac{h^2}{2}(12x_i^2) + \frac{h^3}{6}(24x_i) + \frac{h^4}{24}(24)$$

Given that $h = 0.2$

$$y_{i+1} = y_i + 0.8x_i^3 + 0.2 + 0.24x_i^2 + 0.052x_i + 0.0016$$

Hence, by putting $i = 0, 1, 2, \text{ and } 3$ respectively, we can evaluate y_1, y_2, y_3, y_4 .

The Runge – Kutta Methods

Consider the initial value problem:

$$y' = f(x, y); \quad y(x_0) = y_0$$

Since y' is a function of x , and it can be written as $y(x)$

Then by mean value theorem,

$$y(x_i + h) = y(x_i) + hy'(x_i + \theta h)$$

Where, $0 < \theta < 1$

In our usual notation, this can be written as:

$$y_{i+1} = y_i + hf(x_i + \theta h, y(x_i + \theta h))$$

Now, choosing $\theta = \frac{1}{2}$, we obtain:

$$y_{i+1} = y_i + hf\left(x_i + \frac{h}{2}, y_i + \frac{h}{2}f_i\right)$$

And since Euler's method with spacing $\frac{h}{2}$, this formula may be expressed as:

$$d_1 = hf(x_i, y_i)$$

$$d_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{d_1}{2}\right)$$

Therefore,

$$y_{i+1} = y_i + d_2$$

This is called the second order Runge – Kutta formula.

The third order formula is:

$$d_1 = hf(x_i, y_i)$$

$$d_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{d_1}{2}\right)$$

$$d_3 = hf(x_i + h, y_i + 2d_2 - d_1)$$

Therefore,

$$y_{i+1} = y_i + \frac{1}{6}(d_1 + 4d_2 + d_3)$$

The fourth order Runge – Kutta formula is given as:

$$d_1 = hf(x_i, y_i)$$

$$d_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{d_1}{2}\right)$$

$$d_3 = hf\left(x_i + \frac{h}{2}, y_i + \frac{d_2}{2}\right)$$

$$d_4 = hf(x_i + h, y_i + d_3)$$

Therefore,

$$y_{i+1} = y_i + \frac{1}{6}(d_1 + 2d_2 + 3d_3 + d_4)$$

Example

Solve the initial value problem value using the Runge – Kutta second order method.

$$\frac{dy}{dx} = (1 + x^2)y ; \quad y(0) = 1 ; \quad x = 0(0.2)0.6$$

Solution:

$$f(x, y) = (1 + x^2)y ; \quad x_0 = 0, y_0 = 1, h = 0.2$$

$y_0 = 1$	$y_1 = ?$	$y_2 = ?$	$y_3 = ?$
$x_0 = 0$	$x_1 = 0.2$	$x_2 = 0.4$	$x_3 = 0.6$

To find y_1

$$d_1 = hf(x_i, y_i) = 0.2(1 + x_0^2)y_0$$

$$= 0.2(1)(1) = 0.2$$

$$d_2 = hf\left(x_i + \frac{h}{2}, y_i + \frac{d_1}{2}\right) = hf(0.1, 1.1) = 0.2(1 + 0.01)1.1$$

$$= 0.2222$$

Therefore,

$$y_1 = y_0 + d_2 = 1 + 0.2222$$

$$= 1.2222$$

To find y_2 :

$$\begin{aligned}d_1 &= hf(x_1, y_1) = 0.2(1 + x_1^2)y_1 = 0.2(1 + 0.04)(1.2222) \\&= 0.2542222\end{aligned}$$

$$\begin{aligned}d_2 &= hf\left(x_1 + \frac{h}{2}, y_1 + \frac{d_1}{2}\right) = hf(0.3, 1.349333) = 0.2(1 + 0.09)(1.34933) \\&= 0.2941546\end{aligned}$$

$$\text{Then, } y_2 = y_1 + d_2 = 1.2222 + 0.2941546 = 1.5163768$$

To find y_3

$$\begin{aligned}d_1 &= hf(x_2, y_2) = 0.2(1 + x_2^2)y_2 = 0.2(1 + 0.16)(1.5163768) \\&= 0.3517994\end{aligned}$$

$$\begin{aligned}d_2 &= hf\left(x_2 + \frac{h}{2}, y_2 + \frac{d_1}{2}\right) = hf(0.5, 1.6922785) \\&= 0.4230691\end{aligned}$$

$$\begin{aligned}\text{Then, } y_3 &= y_2 + d_2 = 1.5163768 + 0.4230691 \\&= 1.9394459\end{aligned}$$

Assignment

Solve the problem given below, using the Runge – Kutta fourth order method:

$$\frac{dy}{dx} = (1 + x^2)y ; \quad y(0) = 1 ; \quad x = 0(0.2)0.6$$

CHAPTER EIGHT

NUMERICAL INTEGRATION

Methods:

1. Trapezoidal Formula

$$y = \int_a^b f(x)dx \approx h \left(\frac{y_0 + y_n}{2} + y_1 + y_2 + \dots + y_{n-1} \right)$$

where, $y_i = f(x_i)$, $(i = 0, 1, 2, \dots, n)$

$$h = \frac{b - a}{n}$$

2. Simpson's Formula (Parabola formula)

$$y = \int_a^b f(x)dx \approx \frac{h}{3} [y_0 + y_{2m} + 2(y_2 + y_4 + \dots + y_{2m-2}) + 4(y_1 + y_3 + \dots + y_{2m-1})]$$

$$\text{where } h = \frac{b - a}{n} = \frac{b - a}{2m}$$

3. Newton's Formula ($\frac{3}{8}$ rule)

$$y = \int_a^b f(x)dx \approx \frac{3h}{8} [y_0 + y_{3m} + 2(y_3 + y_6 + \dots + y_{3m-3}) + 3(y_1 + y_2 + y_3 + y_4 + \dots + y_{3m-2}) + y_{3m-1})]$$

$$\text{where, } h = \frac{b - a}{n} = \frac{b - a}{3m}$$

Example 1

Evaluate the integral, employing the trapezoidal rule, for n = 10

$$y = \int_0^1 e^{-x^2} dx$$

Solution:

Form a table of the integrand function

i	x_i	x_i^2	y_i
0	0	0.0	1.0000
1	0.1	0.01	0.9900
2	0.2	0.04	0.9608
3	0.3	0.09	0.9139
4	0.4	0.16	0.8521
5	0.5	0.25	0.7755
6	0.6	0.36	0.6977
7	0.7	0.49	0.6125
8	0.8	0.64	0.5273
9	0.9	0.81	0.4449
10	1.0	1.00	0.3679

Applying the formula;

$$y = \int_a^b f(x) dx \approx h \left(\frac{y_0 + y_n}{2} + y_1 + y_2 + \dots + y_{n-1} \right)$$

We note that $\frac{1}{2} (y_0 + y_{10}) + \sum_{i=1}^9 y_i = 7.4620$

Therefore,

$$y = \int_0^1 e^{-x^2} dx = h * 7.4620 = 0.1 * 7.4620$$

$$\approx 0.746$$

Example 2

Compute the integral; $y = \int_0^1 e^{x^2} dx$ by the Simpson formula, for n = 10

Solution:

Form a table of the function:

			Values of $y_i = e^{x^2}$		
i	x_i	x_i^2	for $i = 0, 10$	for even i	for odd i
0	0	0.00	1.0000		
1	0.1	0.01			1.0101
2	0.2	0.04		1.0408	
3	0.3	0.09			1.0942
4	0.4	0.16		1.1735	
5	0.5	0.25			1.2840
6	0.6	0.36		1.4333	
7	0.7	0.49			1.6323
8	0.8	0.64		1.8965	
9	0.9	0.81			2.2479
10	1.0	1.00	2.7183		
<i>Summation</i>			3.7183	5.5441	7.2685

Applying the Simpson's formula:

$$\int_0^1 e^{x^2} dx \approx \frac{1}{30} [(3.7183) + 2(5.5441) + 4(7.2685)]$$

$$= 1.46268 \approx 1.4627$$

Example 3

Compute the integral, using the Newton's formula for $h = 0.1$

$$\int_0^{0.6} \frac{dx}{1+x}$$

Solution:

$$\text{If } h = 0.1 \text{ then } n = \frac{b-a}{h} = \frac{0.6-0}{0.1} = 6$$

Now form a table of the function:

			Values of $y_i = \frac{1}{1+x_i}$		
i	x_i	$1 + x_i$	for $i = 0, i = 6$	for $i = 3$	for $i = 1,2,4,5$
0	0	1.00	1.0000		
1	0.1	1.10		0.9091	
2	0.2	1.20			0.8333
3	0.3	1.30		0.7692	
4	0.4	1.40			0.7143
5	0.5	1.50			0.6667
6	0.6	1.60			
<i>Summation</i>			1.6250	0.7692	3.1234

Applying the formula, we obtain;

$$y = \int_a^b f(x) dx \approx \frac{3h}{8} [y_0 + y_{3m} + 2(y_3 + y_6 + \dots + y_{3m-3}) + 3(y_1 + y_2 + y_3 + y_4 + \dots + y_{3m-2}) + y_{3m-1})]$$

$$\int_0^{0.6} \frac{dx}{1+x} \approx \frac{3}{8} * 0.1 * (1.6250 + 1.5384 + 9.3702) \approx 0.47001$$

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